Grain surface chemistry in astrophysical objects

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Conclusions and future work

THIS thesis research has focussed on grain surface chemistry in astrophysical objects. In particular, two main questions have been addressed: (1) How do molecular hydrogen molecules form on dust grains? (2) How does grain surface chemistry lead to a complex chemistry as the one detected toward Hot Cores?

The main conclusions are summarized here and an outline of possible follow-up studies is given.

Molecular hydrogen formation in the Universe

Molecular hydrogen is the most abundant molecule in the universe and plays a fundamental role in the interstellar medium. Theoretical arguments suggest that the largest percentage of molecular hydrogen is formed in interstellar space when hydrogen atoms recombine on surfaces of interstellar matter. In this thesis, we developped a model to understand H_2 formation on grain surfaces. This model fully takes into account the presence of both physisorbed (weak bound) and chemisorbed (strong bound) sites on the surface, allows quantum mechanical diffusion as well as thermal hopping for absorbed H atoms. While extended to astrophysical conditions (steady state, low temperatures), simple analytical expressions for H_2 formation can be derived for a wide variety of surfaces, once surface characteristics are determined experimentally. The important result of this model is the efficiency of H_2 formation, already at low temperatures (above 5-10K), and the formation of this molecule on grain surfaces up to grain temperatures of the order of a hundred kelvin.

In another study, we applied the results of the forementioned model to the high redshift Universe. We found that several physical parameters, in particular dust temperature and gas temperature, but not so much dust surface composition, influence the formation rate of H_2. We studied the relative contribution of H_2 formation on dust grains to that of molecular hydrogen formation in the gas phase, through the H^- route. The ratio of formation rates of these two routes depends to a large extent on the dust abundance, on the electron abundance, as well as the relative strength of the FUV (extra-)galactic radiation field. According to our model, for a cosmological evolution of the star formation rate and dust density consistent with the Madau plot, a positive feedback effect on the abundance of H_2 due to the presence of dust grains can occur as early as a redshift of $z \sim 3-5$ which correspond to a dust-to-gas mass ratio as small as 10^{-4}-10^{-3} of the galactic value.

Molecular complexity

The formation of low mass stars such as the Sun remains a complex subject involving numerous physical and chemical processes. Due to advances in observational techniques our present understanding has considerably improved and a coherent picture of how stars are formed is emerging: stars are formed in collapsing, dense clouds of dust, gas, and ice. An early stage of star formation presents a highly obscured protostar, the so-called "Class 0" phase, only visible at far infrared and millimetre wavelengths. The gravitational and rotational energy that is released during the collapse leads to various violent processes. This strongly affects the dynamical, physical and chemical evolution of the material in the surrounding protostellar envelope. During this first phase, the newly formed star heats up its environment, creating a Hot Core region characterized by warm temperature (T$\geq$100K), high densities ($n_H \sim 10^6$ cm^{-3}) and a rich and unique molecular inventory. The molecules present in these objects are complex and saturated species which are not abundant in dark molecular clouds. This rich chemistry is generally attributed to grain surface chemistry and mantle evaporation processes. Previously, Hot Cores were exclusively associated with regions of massive star formation. In this thesis, we present observations showing the existence of a Hot Core in the solar type protostar IRAS16293-2442, located in the ρ Oph complex at 120 pc of distance. Indeed, our observations revealed an extremely rich organic inventory in this source with abundant amounts of complex O and N-bearing molecules such as formic acid, HCOOH, acetaldehyde, CH_3CHO, methyl formate, CH_3OCHO, dimethyl ether, CH_3OCH_3 , acetic acid, CH_3COOH, methyl cyanide, CH_3CN, ethyl cyanide, C_2H_3CN and propyne, CH_3CCH. The chemical composition of the Hot Core around this low mass young stellar object presents numerous differences in comparison to those around massive protostars. It is clear that further studies of the molecular inventory of low mass young stellar objects are urgently needed to provide important information on the detailed chemical routes involved in the drive towards molecular complexity, as well as to shed light on the origin of the molecular composition of the early Solar System and the organic reservoir available to life on the early Earth.

Future work

The results presented in this thesis highlight a number of new issues that should be further explored by future research studies and future space missions. One of these objectives is the development of a theoretical model of grain surface chemistry coupled with gas phase chemistry, aiming at understanding the chemical characteristics and evolution of low mass Hot Cores. This model adapted from Caselli, et al. 1993, will be extended significantly to low mass Hot Core objects. It follows the chemical evolution of collapsing clouds, until the end of the protostar accretion phase. In this final stage, the temperature increases and the grain mantles evaporate into the gas phase. In this model, a combination of hot gas chemistry and grain surface chemistry is considered and the composition of the gas is monitored. This model, adapted to the physical and chemical conditions of low mass Hot Cores, will be implemented for hydrogenation and deuteration of specific molecules, and will study the different pathways that lead to the observed chemical complexity. To do this, the model will determine the contribution from both gas phase and grain surface chemistry routes in the formation of these complex molecules. The model we propose to build should thus permit a better understanding of the role of surface and gas phase chemistry in these objects. It should also provide an adequate chemical network to understand low mass Hot Cores and their chemical differentiation with respect to massive Hot Cores. In that sense, such a tool could be used as a chemical "clock" that indicates the evolutionary state of the embedded protostar. One second objective is to check the most significant features of our theoretical predictions against real observations of low mass Hot Cores. The molecular inventory of these objects is necessary to point out potential chemical differentiations between Hot Cores. For this purpose, several observational campaigns are already planned at mid- to high spatial resolution, using respectively the IRAM 30-m telescope (Spain) and the IRAM Plateau de Bure interferometer (France). In particular, a complete spectral survey of IRAS16293-2422 will be conducted. This will provide a "complete" inventory of the molecular complexity of this prototypical Class 0 protostar. In addition, a sample of seven young stellar objects has been selected as candidates for follow-up observations aiming at assessing the chemistry of these low mass Hot Cores.

Figure 6.1–. Herschel Space Observatory (HSO)

In addition, this possible issue will actively contribute to the scientific preparation for HIFI. HIFI is the heterodyne instrument on board of the Herschel Space Observatory (HSO), an ESA project to be launched in 2007. This instrument represents our best chance to address some fondamental aspects of the star formation for the years to come. This mission will open up the submillimeter window in the frequency range between 500 and 2000 GHz, which was up to now unreachable from the ground due to terrestrial astmosphere extinction. This frequency range provides a particularly good probe of warm gas around young protostars.

In particular, the heterodyne instrument HIFI will allow observation at both high spectral resolution and high sensitivity. One of the key programs of this instrument will focus on the study of the formation of stars, from low to high mass, with particular emphasis on the chemistry and energetics that govern their formation. The preparation of simulation and analysis tools prior to launch is a mandatory effort to guarantee the most efficient outcomes of such a unique mission. This preparation work has already started under the leadership of A. Tielens (Groningen) for the HIFI consortium, and M. Walmsley (Arcetri), C. Ceccarelli (Grenoble) and P. Caselli (Arcetri) regarding the specific area of star formation.